A Breakthrough Is Something You Don't See Coming

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Published in:
Progress in Materials Science

Progress in Materials Science 56 (2011) 573–576

Contents lists available at ScienceDirect

Progress in Materials Science

journal homepage: www.elsevier.com/locate/pmatsci

Preface

"A Breakthrough Is Something You Don't See Coming"

According to the Oxford Dictionary of English a 'Festschrift' is a compilation of writings published in honor of a colleague and scholar. For this special issue of Progress in Materials Science our definition will be extended to 'a collection of elegant essays contributed by a group of scholars to an older and even greater scholar at a milestone in his life'. Within this revised convention: to recognize Vaclav Vitek's influential contributions to computational materials science and engineering upon the occasion of his 70th birthday "The Vaclav Vitek Honorary Symposium on Crystal Defects, Computational Materials Science and Applications" was held during the TMS 2010 139th Annual Meeting & Exhibition in Seattle, USA, February 14–18, 2010. The goal of the organizers, Mo Li, (Georgia Institute of Tech), David Srolovitz (Institute for High Performance Computing, Singapore), Adrian Sutton (Imperial College, London), Vaclav Paidar (Institute of Physics, Prague) and myself (Applied Physics, University of Groningen, the Netherlands) was to bring together scientists from across the areas of materials science that have been impacted by Professor Vitek's work. The enthusiasm in the response was overwhelming, illustrated by about 20 invited papers and more than 100 presentations in total. The range of topics represented in this special issue of Progress in Materials Science is a sample of Vaclav Vitek's scientific interests and collaborators. As an introduction to this Festschrift, a brief resume seems appropriate.

Vaclav Vitek, Professor of Materials Science and Engineering at the University of Pennsylvania in Philadelphia, was born in Olomouc in 1940. The ancient town of Olomouc being the ecclesiastical

doi:10.1016/j.pmatsci.2011.01.001

metropolis of Moravia in the east of the Czech Republic dates back to the 10th century AD when it became an important trade crossing-point. After his studies in physics at the Charles University in Prague Vaclav Vitek received his PhD in 1966 at the Institute of Physics of the Czechoslovak Academy of Sciences. His thesis supervisor was František Kroupa (1925–2009), well known to all of us working in the field of dislocations and defects in metallic systems. He introduced and encouraged Vaclav Vitek to the study of the mechanical behavior of materials and predicted that with advancements of computers we should be able to get to atomic level studies of materials deformation. Indeed, to a certain extent that prophesy became true. In 1967 Vaclav Vitek went as a post-doctoral Fellow to the Department of Materials at Oxford University, England, headed by Sir Peter Hirsch and Jack Christian. It was as a postdoc at Oxford that Vaclav Vitek wrote his most cited paper, which introduced the concept of the gamma-surface (V. Vitek, Phil. Mag. 18, (1968) p. 773).

After the Soviet invasion of Czechoslovakia he decided to remain in the United Kingdom and stayed until 1975 at Oxford as a Research Associate at the Department of Materials and Research Fellow of the Wolfson College. In 1975 he became the Principal Research Officer at the Central Electricity Research Laboratories, Leatherhead, England. During this time he acquired the British nationality by naturalization. As a result of a concerted action of Charlie McMahon, Dave Pope and Campbell Laird to the Dean's office at Penn, Vaclav Vitek was invited in 1978 to become a Full Professor at the University of Pennsylvania where he remains until today. During this time he held several visiting professorships: Theoretical Physics Division, AERE, Harwell, U. K. (1985); Department of Applied Physics, University of Groningen, the Netherlands (1985–1986); Department of Physics, École Polytechnique Fédérale de Lausanne, Switzerland (1989); Max-Planck-Institut für Metallforschung, Stuttgart, Germany (1992–1993); Korean Institute of Science and Technology, Taejon, Korea (2003); Seoul National University, Seoul, Korea (2004). He became a naturalized US citizen in 1984.

In contrast to present habits in the scientific community, Vaclav Vitek has been working on very similar problems in materials science and engineering for his whole career of more than 40 years and it is noteworthy with admiration that he has resisted jumping from one fashion, or trend and hype to the next. Indeed, today it takes a pretty strong personality not to grasp the low hanging fruit when pursuing the more principal and essential problems in materials science. According to Marc Cawkwell, a recent PhD student, the viewpoint of Vaclav Vitek is that solving really fundamental problems in materials takes time and it is rather silly to expect that these fundamental questions can be answered within a short period. A beautiful illustration of this is the work in Science dealing with the origin of brittle failure of Iridium (Marc J. Cawkwell, Duc Nguyen-Manh, Christopher Woodward, David G. Pettifor and Vaclav Vitek, Science 309, 1059–1062 (2005)).

With this approach, Vaclav Vitek has gained the unbridled respect of his peers that has been reflected in the numerous accolades showered upon him. These have included being named ASM International Fellow and TMS Fellow, the organizations highest recognitions, and being inducted into the US National Academy of Engineering in 2006. For his contributions to the science of materials, he was honored by several awards: Pfeil Medal of The Metals Society (London) in 1982, Alexander von Humboldt Senior Scientist Award (Germany) in 1991, NEDO Research Award (Japan) in 1992, Acta Metallurgica Gold Medal in 1996, Honorary Doctorate of the Technical University of Brno in 1999, Ernst Mach Medal in Physical Sciences awarded by the Czech Academy of Sciences in 1999. He presented numerous invited lectures at international conferences, universities and research establishments, published over two hundred original papers in peer-reviewed journals, close to fifty invited papers and reviews and more than hundred papers in various conference proceedings. He also edited three books dealing with atomic level studies of defects in materials and is a member of editorial boards of several international journals in the field of materials science.

His interests are at least in three distinct areas of materials research that are also reflected in this Festschrift. The necessary precursor of any atomistic study is a physically based description of atomic interactions that reflects correctly the principal aspects of bonding. As a consequence, the topic of atomic interaction functions for atomistic computer modeling is central in the work of Vaclav Vitek, built upon a fruitful collaboration with David Pettifor in Oxford when developing bond-order potentials for real systems. The work ranges from many-body central-force potentials to bond-order potentials that are capable to reflect correctly the mixture of metallic and covalent bonding

encountered in many complex structural and functional materials. These aspects will be touched upon in the contribution by Všianská and Šob. The second category of activities of Vaclav Vitek concentrates on atomic level behavior of dislocations in transition metals, in intermetallic compounds and atomic level description of defects in metallic glasses. In this research he develops physically based constitutive models for macroscopic analyses of the plastic flow. In particular, the fundamental explanations of the anomalous temperature dependence of the yield stress and related orientational dependencies in ordered $L1_2$ compounds (V. Paidar, D.P. Pope and V. Vitek, Acta Metall. 32, (1984) p. 435) made a tremendous impact to the field of dislocations, including to the field of engineering applications of high-temperature resistant intermetallic compounds in general. His approach of multiscale modeling links the atomic level properties of defects with macroscopic plastic behavior and builds a bridge between basic physics and properties of engineering materials. The state-of-the-art of these aspects are discussed in the contributions by Bassani and Racherla, Hirth and Pond, Greer and De Hosson, Paidar, Sauzay and Kubin, Takeuchi and Edagawa, Egami. The third research topic dates back to his monumental contributions on structural unit models together with his first PhD student Adrian Sutton (A.P. Sutton and V. Vitek, Phil. Trans. Roy. Soc. A309, (1983) pp. 1, 37, 55) and deals with interfaces and grain boundaries. At present, using computer simulations, Vaclav Vitek investigates the atomic and electronic structure as well as properties such as interfacial cohesion, diffusion, formation of unusual interfacial phases, interaction with dislocations and interfacial chemistry related to segregation. The calculations range from ab initio DFT based electronic structure calculations, real space tight-binding methods, to state of the art empirical approaches allowing modeling of very large systems. The modeling is synergistically linked with experimental studies, e.g. electron microscopy. These topics will be treated in this Festschrift by Všianská and Šob, Mo Li and Tao Xu, Paidar, Hirth and Pond.

As a flashback over 40 years of computational materials science, one should realize that in the early days Vaclav Vitek was exploring largely uncharted and fully unknown territory as he toiled on atomistic simulation of dislocation cores. At that time, one computer served the entire university of Oxford, reminds Adrian Sutton us, and as a post-doctoral fellow, the only way Vaclav Vitek could ensure access to it for his studies was to spend a lot of nights in the computer center. So it was in the wee hours of the morning at Oxford University in the late 1960s, beginning of the 1970s, that the field of dislocation core simulations was emerging and that fundamental insights in plastic deformation of bcc metals were attained as prophesied and hoped for by František Kroupa. The combination of passion during marathon late-night sessions in Oxford and computer equipment, excellent in those days but primitive for our present standards, helped to lay the groundwork for today's field of computational materials science. In the words of his very first PhD students, Adrian Sutton and David Srolovitz: "When Vasek began his simulations of screw dislocations in the sixties, there were very few people anywhere in the world engaged in such work. Metallurgy, as materials science was known then, was largely an empirical subject, dominated by experimentalists with a few theorists working with pencils and paper. Today, we regard computational materials science as one of the central pillars of the subject, and there are thousands of people engaged in the pursuit. Vasek has contributed directly to that transformation through his own seminal research. But he has also mentored others who have gone onto become leaders of the field in their own right. He is a real father figure in computational materials science."

After having contributed so vigorously to the growth and knowledge base of computational materials science and engineering over the years, Vaclav Vitek said in the End Notes interview with Lynne Robinson, JoM, October 2009, page 80 "that predicting truly new directions in the field is almost impossible. If I were able to tell what the next exciting advance will be, it would not be a breakthrough. A breakthrough is something that you don't see coming."

It is a pleasure to acknowledge and to thank Vaclav Vitek for his drive and enthusiasm, for his scholarly approach to science and also to society, for his seminal contributions and impetus to computational materials science and engineering, for his guidance and impact on the numerous young scientists who have studied with him and for his friendship over the many years we received from him and his late wife Luda. On behalf of all friends: sincere congratulations go to Vaclav Vitek and the authors wish all fellow scholars the brightest joys of studying the elegant essays laid down in this Festschrift.

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